A Noniterative Model for CO_2-H_2O Mutual Solubilities in Chloride Brines

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RESEARCH OBJECTIVES

The objective of this study was to develop a numerically efficient model to compute the mutual solubilities of CO_2 and H_2O in chloride brines, for applications to CO_2 geologic sequestration studies. One specific goal was to avoid degrading the performance of numerical fluid-flow simulations when using such a model.

APPROACH

We previously developed a numerically efficient thermodynamic model for phase partitioning without salt effects. This model was shown to provide an excellent match to experimental data in the range 12–100°C and up to 600 bar. Here, the model is extended to NaCl and $CaCl_2$ solutions by including an activity coefficient for aqueous CO_2, and taking the activity of water as its mole fraction on the basis of a fully ionized salt. Several published activity coefficient formulations were evaluated, two of them based on a Pitzer formulation and providing best results (Figure 1).

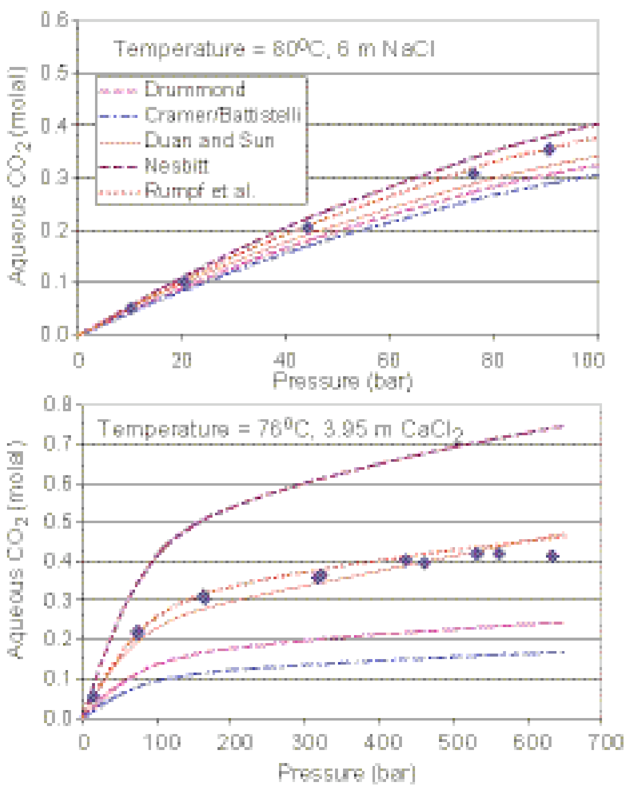

Figure 1. Measured (symbols) versus predicted (lines) CO_2 solubilities using five different activity coefficient models

ACCOMPLISHMENTS

For solutions up to 6 molal NaCl and 4 molal $CaCl_2$ (Figure 1), the best activity coefficient formulations yield calculated CO_2 solubilities within less than 7% (root-mean-square error) of experimental data. Thus, the new model allows computing mutual solubilities in a noniterative manner and with an accuracy typically within experimental uncertainty.

SIGNIFICANCE OF FINDINGS

Previously published models involve complex correlations requiring an iterative solution and/or do not cover temperatures below ~100°C at high pressures. The approach followed here is noniterative, thus numerically efficient, and reproduces experimental solubilities with sufficient accuracy for the study of geologic CO_2 disposal.

RELATED PUBLICATIONS

Spycher, N., K. Pruess, and J. Ennis-King, CO_2-H_2O mixtures in the geological sequestration of CO_2. I. Assessment and calculation of mutual solubilities from 12 to 100°C and up to 600 bar. Geochimica et Cosmochimica Acta, 67, 3015–3031, 2003. Berkeley Lab Report LBNL-50991.

Spycher, N., and K. Pruess, CO_2-H_2O mixtures in the geological sequestration of CO_2. II. Partitioning in chloride brines at 12 to 100°C and up to 600 bar. Geochimica et Cosmochimica Acta 69 (13), 3309-3320, doi:10.1016j.gca.2005.01.015, 2005. Berkeley Lab Report LBNL-56334.

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